GAS COMPOSITION CALCULATION FOR THE IN SITU
GASIFICATION OF THIN SEAMS AND THE APPROACH TO MODELING

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INTRODUCTION

The Appalachian region contains numerous coal seams which are under 60 inches
in thickness. A portion of this coal is usually recovered by Auger mining tech-
niques after contour stripping. At least fifty percent of the remaining coal may
be gasified to produce a low Btu fuel. The application of underground gasification
to very thin seams (below 40 inches in thickness) is limited by the reduction of
the heating value of the gas. This reduction is caused by an excessive heat loss
to the surrounding strata.   The purpose of this work was to evaluate the pertinent
factors affecting the gas composition and the limitations of modeling calculations.
The logical sequences leading to a gas composition model and the estimation of the
temperature profile in the gasification zone were presented. The available litera-
ture data related to the various calculation techniques were also quoted.

PARAMETERS AFFECTING THE GAS COMPOSITION

The total heat losses during the in situ gasification affect significantly the
gas composition and its heating value. A heat balance results in a temperature
profile of the gasification zone. One modeling approach is to calculate the gas
composition and compare this composition to the data obtained from the experimental
tests. A second approach involves a prediction of the temperature profile of the
gasification zone. The gasification of coal seams having a thickness from one or
more meters is considered here. The combustible gases formed during the underground
forward gasification mode are obtained by pyrolitic coal decomposition superimposed
upon the gasification products. As far as the gasification is concerned, the
reaction of coal with the steam and/or hydrogen is of paramount importance because
this is the main reaction which produces a gaseous burnable product of heating value
above 100 Btu/SCF. The ratio of the total amount of water (in the form of coal
moisture plus inflow of water or steam) to the supplied amount of oxygen seems to
be a predominant factor in maximizing gas heating value for the defined level of
total heat losses.

In general, the gas composition of the underground gasified coal depends on
the volatile content, the seam moisture, the blast air moisture content, and the
chemical reactivity of the coke. The gasification efficiency and combustion
stability are sensitive [Stewart et al. (24)] to the optimum combination of the
coal seam moisture and of blast air moisture.

The reactivity of a particular coal is a function of the chemical properties
of its organic and mineral constituents and of the physical structure of the coal;
generally, it is observed that the coal reactivity in gasification increases with
decreasing coal rank and is proportional to the internal surface area [Schora, F.
(23)]. When experimental values for the relative low-rate gasification reactivity
factors (f_o) are not available; values for many coal [Johnson, S. L. (15)] may
be estimated from the following equation: $f_o = 6.2 \, y \, (1-y)$ where y is the mass
faction of total carbon in the original coal on a dry ash-free basis. The condi-
tions during a pyrolysis of the coal affect the physical nature of the char and

its reactivity. In the temperature range 600–700° C, where the apparent activation energy is high (80–70 kcal/mole), the reaction rate is low and the composition of gas is limited by the kinetic reaction rate; in the temperature range 700–750° C the diffusion process through the pore structure is a limiting factor. However, [Limears et al. (19)] have shown that for some coal types the particle size has nearly no effect upon the char reaction rate.

In general, the rate of the steam-hydrogen reaction with the coal depends on many variables such as: temperature, pressure, character of the coal solid surface and the amount of volatile matter in coal. The first stage of the reaction is rapid and is related to the gasification of the carbon portion included in the volatile matter. The low reactivity coal portion is the residual, carbonaceous coke. This stage is usually denoted as (1) $C* + H_2O \rightarrow CO + H_2$ and (2) $H_2 + H_2O + 2C \rightleftarrows CO + CH_4$ where $C*$ is the reactive carbon in the volatile matter. Most coals are made up of a number of marcels which differ in their reactivity. [Davis et al. (19)] found a reactivity order fusian < durain < vitrain.

The endothermic reaction of steam with carbon is of primary importance. These endothermic reactions are maintained by the enothermic oxidation reaction of carbon and oxygen.

The higher activation energy observed for the carbon reaction with the steam-hydrogen mixture indicated an inhibiting effect of hydrogen (and/or methane) on the char-steam reaction. The reactivity of such a mixture was proportional to the steam pressure raised to the 0.93 power [Johnson (15)].

[Young et al. (30)] reported on the effect of the steam upon the methane production and the shift reaction under conditions that are similar to those of underground gasification. Wyodak and Hanna char was used. No carbon monoxide was detected for the steam-char gasification process to indicate that the water shift reaction $CO + H_2O \rightarrow CO_2 + H_2$ had taken place. The gas shift reaction was probably catalized by the ash content in the char. Introduction of steam during the pyrolysis period doubled the rate of methane production. The rate of methane production was 20 percent of that of carbon dioxide. Russian investigators have reported similar data.

Experimental kinetic data indicate that we will not be able to use equilibrium compositions in making our modeling calculations.

We compare below the equilibrium composition of wet water gas at 900° C and 1000° C and the kinetic data of the reaction between the flowing gas (0.7 - 0.9 m/sec) and the carbon particles 2-3 mm. in the reactor (data according to [Kaftawov et al. (17)]).

TEMPERATURE	EQUILIBRIUM COMPOSITION DATA		COMPOSITION ACCORDING TO KINETIC DATA			
	%CO	%H$_2$	%CO$_2$	%CO	%H$_2$	%CH$_4$
900° C (1652° F)	45	50	10.1	34.6	55.2	0.1
1000° C (1832° F)	50	50	8.8	38.1	52.9	0.2

The equilibrium constant may be calculated from the Gibbs free energy (G): $\Delta G = R T \ln k$ where $\Delta G = \Delta H - T \Delta S$. The correlation between the equilibrium constant and the temperature is expressed usually by the equation (p = const):

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$$\ell nk \;=\; \frac{1}{R}\int \frac{\Delta H}{T^2}\, dT \;+\; a \quad \text{(where a is an integration constant).}$$

Several difficulties are encountered in a discussion of the kinetics of coal gasification. Since the effects of coal devolatilization on the product gas rates are important up to temperatures between 600–700° C, usually only the data above 700°C are analyzed to obtain the kinetic constant. Laboratory experiments show that during the coal burn-off _versus_ time studies a gradual induction period is followed by a region in which burn-off increased with a time. Instantaneous re-activity (R) may be calculated from the equation:

$$R_t \;=\; (\frac{1}{W_E})\;(\frac{dw}{dt})$$

where W_e is the weight of the unreacted char on a dry-ash free basis and $\frac{dw}{dt}$ is the slope of the burn-off versus time. For the reaction in the air R_t increases and often W_E is replaced by W_0 (starting weight) and $\frac{dw}{dt}$ is taken for the maximum rate of weight loss.

The first principal reaction which occurs during the underground coal gasification process is the pyrolysis. The rate of pyrolysis as well as the amount and composition of the volatile products from a given sample of coal or char depends on the rate of heating, the final decomposition temperature, the vapor residence time and the environmental conditions such as applied pressure, particle size, coal type, etc. under which the pyrolysis takes place.

Normally pyrolysis starts at about 350°–400° C and is completed at about 1000° C. The reactivity with steam, oxygen, hydrogen or carbon dioxide during the pyrolysis of coal is mainly a function of the volatile matter and the rate of heating.

GASIFICATION RATE OF CHAR IN THE CARBON DIOXIDE ATMOSPHERE

The reaction between the char and carbon dioxide is hardly detectable below the temperature 800–900° C. According to Wen, C. Y. et al. (4) the activation energy is about 59.26 kcal/mole which indicates chemical-reaction control. The following mechanism was proposed by Walker (28):

$$C + CO_{2(g)} \xrightarrow{\;T_1\;} CO_{(a)} + CO-_{(g)}$$

$$CO_{(a)} \xrightarrow{\;T_2\;} CO_{(g)}$$
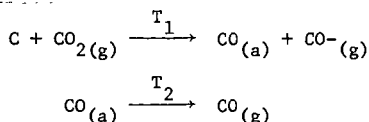
Experimental data indicated that the order of reaction with respect to CO_2 can be assumed to be unity up to about one atmosphere pressure. However, at higher temperatures, the diffusion resistance within the solid particle may become significant and therefore an effectiveness factor must be introduced for such cases.

According to Wen et al. (4) the rate of the char-carbon dioxide reaction is found to depend on the coal origin more than on the gasification scheme used. The various rate characteristics of coals and chars are apparently due to the difference in their pore characteristics.

GASIFICATION RATE OF CHAR ON OXYGEN-ATMOSPHERE

The reaction rate in the temperature range 424–576° C using air was determined recently by C. Y. Wen et al. (4). The rate of reaction showed a maximum at a conversion of 10–50 percent; the maximum depended on the sample used. The observed

maximum reaction rate, dx/dt, was 1.67×10^{-3} sec^{-1}. Under these conditions the reactivity of the char is determined by chemical kinetics and depends more on the extent of the gasification of the char rather than on the parent coal.

In the temperature range 834-1106° C, the raction rates appear to correspond to a film-diffusion control regime. The rates do not change significantly with conversion degree until about 80 percent conversion is reached. Assuming a spherical particle shape, the average rate at 1000° C was 1.8×10^{-6} g/cm^{2}s atm. A nitrogen-air mixture was used as the low oxygen concentration source.

THE GASIFICATION RATE OF CHAR IN THE HYDROGEN-ATMOSPHERE

A. Tomite et al. (26) investigated the reactivity of a char which was prepared at 1000° C. Usually the reactivity profile of a majority of the chars shows some slow induction period followed by a rate increase. The reaction rate generally increases as the rank of the parent coal decreases. Removal of mineral matter profoundly affects the reactivity profile of chars. In most cases the reaction rate decreases with mineral-matter removal.

The pseudo-activation energy changes from 150 kcal/mole to about 213 kcal/mole with increased conversion of the char.

According to Feistel et al. (6) the kinetic constant of hydrogasification is strongly affected by the hydrogen pressure and was expressed by the equation:

$$K_{H2} = \frac{0.00402 \text{ exp. } (-5200/T) \ P^2_{H_2}}{1 + 0.000648 \text{ exp. } (4100/T) \ P_{H_2}}$$

The gasification rate with steam-hydrogen, resulted in the experimental equation, which shows a significant effect of the temperature upon the gasification rate.

The activation energy for the kinetic equation rate was 33,600 cal/ mole and the frequency factor was 2.51×10^4 ℓ/min.

THE REACTION RATE OF CHAR IN STEAM ATMOSPHERE

Linares et al. (19) found that in general the char reactivity was related to the steam reaction and decreased with an increase in the rank of the parent coal. However, a considerable spread in reactivities of char produced from coals of similar rank was observed. Removed of mineral matter diminished the char reactivity but the removal of mineral matter also resulted in a profound change in the surface area and porosity. The influence of each of these variables is difficult to access. Below 890° C the reaction is chemically controlled with an apparent activation energy of 42 kcal/mole. Above 890° C, the reaction is diffusion controlled and has an activation energy of 18 kcal/mole. The reaction rate was found to be proportional to steam pressure raised to the 0.60 power.

The rate of gasification of bituminous coal in the ($H_2O - H_2$) mixture in the temperature range 700-1100° C was investigated by Feistel et al. (6). The kinetic constant for steam decomposition was a function of steam pressure and temperature. The rate of reaction for a pressure higher than 10 atm. was described as:

$$\frac{dx_B}{dt} = K (1-x_B)$$

where x_B is base carbon conversion degree; t-time; k-kinetic constant

$$k_{H_2O} = \frac{1.88 \times 10^6 \exp\,(-2.24 \times 10^4/T)\ P_{H_2O}}{(1 + 1.56 \times 10^5 \exp\,(-1.65 \times 10^4/T)\ P_{H_2O}}$$

$$x_B = \frac{\text{base carbon gasified}}{\text{base carbon in feed coal char}} \text{ (according to Johnson)}$$

THE CHAR REACTIONS IN THE CONDITIONS OF UNDERGROUND GASIFICATION

One possible approach is to calculate the residence time of the char in the high temperature zone of 1500-1800° F. The thickness of the coke zone (coal with 10 percent seam moisture) would be about 0.5 m; for the brown coal at 50 percent moisture this is about 15 cm assuming the advance rate of burning zone about 0.1 x 10^{-5} m/sec. The obtained residence time (40-130 hour range) implies that the seam moisture and volatile content are more significant factors than that of char reactivity upon the overall reaction rate.

THE EFFECT OF THE BLAST INTENSITY AND GASIFICATION ZONE ADVANCEMENT RATE ON THE HEATING VALUE OF PRODUCED GAS

A Russian investigation [Ludin et al. (20)] has shown that the optimum blast rate depends on the thickness of the coal seams. It was explained that the thicker seams have a larger water intrusion rate than the thinner seams. If air is used as the blast; there is an optimum water to air ratio that gives a maximum heating value of produced gas. On the other hand, it was observed the gasification front advancement increased with the higher blast rate. Therefore a certain gasification front advancement rate will correspond to the optimum gas heating value.

THE EFFECT OF THE PEAK GASIFICATION TEMPERATURE UPON THE HEATING VALUE OF THE GAS PRODUCED

The lower concentration of hydrogen caused by the lower temperature gasification does not necessarily lead to a low Btu product gas since a higher methane yield may be obtained in some cases. For example, Gregg et al. (10) found, during some underground tests, 6.3 percent of methane in the gas produced. Fisher et al. (7) made the observation that the presence of steam resulted in a higher concentration of methane in the produced gas. It could be explained that either the steam promotes the reaction of hydrogen and char or the following methanation reaction $CO + 3H_2 \rightleftharpoons CH_4$ occurs. This methanation reaction could be catalyzed by the mineral matter in the char.

INSTABILITY AND UNCERTAINTY FACTORS IN THE UNDERGROUND GASIFICATION MODELING

The following factors would lead to instability of the gasification process and may result in a large modeling error:

1. Change in coal and strata permeability.

2. Rapid water influx. The water may intrude upstream and go through the combustion zone or it may intrude downstream of the combustion zone. In theory an optimum water instrusion exists for any air blast injection. In practice of the gasification usually has a higher water instrusion rate than desirable and operates on the water rich side of optimum.

3. Rapid channeling of gasification process.

4. Rapid gas or air leakage to the strata.

The purpose of this study is to formulate a specific theoretical description of the forward combustion process of thin coal seams (one to several meters thick-

ness) and to establish the base which would allow to compare the model prediction to the eventual results of the field tests. It seems to be worthwhile to mention a few recent publications relating to the in situ gasification modeling. Different methods of gasification and various geological formation lead to different mathematical models. For example modeling were presented by Kotowski (18) and by Gunn and Whitman (12) in the study of reverse and forward combustion. Thorsnes described the evaluation of thermal front measurements and pressure drop versus flow rate. The longwall generator modeling was reported by Sawer and Shuck (22). Some preliminary analysis was given by Gidaspow (9). The practical purpose of underground gasification modeling is to be able to predict the gas composition and permit the development of improved gasification control strategies. The experimental data [Yauagimoto (29)] have shown a significant effect of the gasification zone temperature upon the gas composition. It seems to be difficult to perform an adequate heat balance and to calculate the resulting temperature of the gasification zone considering such phenomena as: thermoplastic behavior as the coal is heated through a certain temperature; porous coke structure, contact area between the flowing gas and gassified coal etc. Therefore the measurements of the gasification zone temperature of the thin seams has been proposed. The equilibrium data calculated for the system volotile – gases from carbon reacting with oxygen, carbon dioxide etc. at the determined temperature, superimposed by the gas composition resulting from the kinetic of char burn out and shift reaction would give the resulting composition of produced gas.

MODELING OF GAS COMPOSITION FOR THE IN SITU GASIFICATION

The logical objectives of fitting equations to experimental data are twofold: to estimate the effect for each of the independent variables and to be able to predict the responses. The preliminary examination of experimental data should lead to:

1. Ordering (in the space or time)

   a. List and magnitude of independent variables
   b. Locate the clusters for estimation of error

2. Plotting

   a. Factor or variable space
   b. Time sequences

The next stage is the construction of specific equations according to the experimental data.

The calculation of gas composition requires a listing of independent experimental variables, as below:

1. Rate of air blast (and the oxygen concentration in the case of air enrichment). This factor is interrelated to the rate of gas production; temperature profile and flame front velocity.

2. Total rate of water moisture supply consisting of coal moisture; blast air moisture and water influx. This is obtained from the total mass balance and measurements.

3. Composition and rate of gas production.

4. Rate of carbon combustion (calculated from point 3.)

5. Coal properties such as moisture, ash, content of volatile, caloric value, conductivity.

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6. Coal combustion characterization such as char reactivity, rate of pyrolysis reaction.

7. Temperature profile of the gasification zone with velocity flame front. The temperature profile follows from the total energy balance. Yanagimoto et al. (29) observed that the calorific value of the gas produced is sensitive to the combustion temperature of underground gasification.

The calculation program is presented below:

100 Mass balance of oxygen and total water. Water influx and air leakage (from material balance). Estimated cluster of errors.

200 The reaction rate and resulting gas composition at the equivalent average temperature of the gasification zone.

201 Pyrolysis of coal and the tar and gas composition derivated from Kinetic equations.

202 Rapid reaction (oxygen, hydrogen, steam) with volatile carbon. Gas composition derivated from equilibrium data.

203 Char reaction with gas phase (oxygen, carbon dioxide, steam). Gas composition derivated from kinetic data. The conversion reaction.

204 Calculation the resulting carbon monoxide, hydrogen and carbon dioxide concentration.

300 Energy balance and the temperature profile.

301 The general energy balance of the solid phase.

302 Heat sink by conduction for surrounding materials.

303 Heat sink by convection to the flowing gases.

304 Heat losses to the ash.

305 Heat used for the water-steam system.

306 Dependent factor: rate of combustion.

307 Problems related to the boundary conditions.

100 The conservation of mass equations for oxygen and total water would be as follows:

[Rate of oxygen (water) mass in]$_1$ – [Rate of oxygen (Water) mass out]$_2$ + [Rate of generation of oxygen (water mass]$_3$ – [Rate of accumulation of oxygen (water mass]$_4$ = 0

Due considerations have to be given for the moisture content of the air; the gasified coal; soil or rock; the strata of the roof in the area of gasified coal; and gravity influx of water respectively as well as the moisture dissociated in the heterogeneous reaction zone and the undissociated moisture in the heterogenous reaction zone). The formula to calculate these water types has been summarized by Kalashinitkov et al. (16). The mass balance of water (being in a form of coal moisture; the water influx and blast moisture) and its discrepancy would show the magnitude of seam water influx and the rate of steam decomposition rate. The continuity equation for these mass balances could be presented as follows:

$$\frac{\partial}{\partial X} (\Delta \text{ mass}) + \Phi m \cdot r + \frac{\partial}{\partial time} (\phi_m \cdot \Delta \text{ mass}) = \text{const.}$$

where Δm can be calculated as the weight fraction of the component in the injected air and $\Phi m \cdot r$ is an oxygen (water) reaction rate function. The mass balance of

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oxygen and its discrepancy would indicate the gas (air) leakage rate and the rate of steam decomposition due to the reactios, e.g.,

$$H_2O + C \rightarrow CO + H_2$$
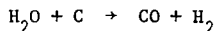
200 The kinetic data concerning the coal devolatilization (pyrolysis) and the combustion of the matter devolatilized from coal should be applied if reliable prediction is to be obtained.

201 The kinetic rate (r) of coal pyrolisis under non-isothermal conditions can be described by two functions:

$r = \dfrac{d\alpha}{dt} = K(T) \, \Phi(\alpha)$ where $\quad a = \dfrac{Vt}{V\infty}$, Vt is the volume of the product in time t and $V\infty$ is the final product volume attained at the end of the reaction. The function $K(T)$ is only temperature dependent, while (α) is a function of the instantaneous phase composition. Using the Arrhenius equation one may obtain the final equation in which the rate of gas production is expressed as follows:

$$\frac{dv}{dt} = \frac{Av\infty}{c} \; \exp \; \frac{-E}{RT} - \frac{A}{C} \; \frac{RT^2}{E} \; e^{-E/RT}$$

The heating rate is denoted here as $c = \dfrac{dT}{dt}$. As an example we use the following experimentally determined kinetic parameters (according to Campbell (2) for subbituminous coal types).

		KINETIC PARAMETERS	
GAS	PEAK AREA %	A (min^{-1})	E^b (Kcal/mole)
H_2	100	1.2×10^3	22.3
CH_4	32.3	1.0×10^7	31.0
CO_2	53.6	3.3×10^4	19.5
CO	30	3.3×10^3	18.0

Pyrolysis of the larger coal particles was described by Forrester (8).

202 The devolatilized compounds, resulting from the coal pyrolysis, burn with oxygen. The reaction rate of volatile compound is very high in the range of 0.5–2 sec. depending on the temperature of the gasification zone. Therefore, the assumption that the equilibrium composition is formed in this zone, seems to be justified. When the state of the system is such that $\Delta G = 0$ no process will occur and the system is at equilibrium. For a system consisting of n-species $\Delta G = \Sigma \, Ni \, \Delta gi$ where Ni is the number of moles of i and Δgi is the molar specific Gibbs function for species i.

If the Gibbs function has the minimum value then for any complete set of independent reaction

$$\frac{\partial \, \Delta G}{\partial \, \epsilon_i} = \sum_{j=1}^{n} \frac{\partial \, \Delta G}{\partial \, Ni} \; \frac{\partial \, Ni}{\partial \, \epsilon_i} = \sum_{j=1}^{n} (\beta_{ij} - \alpha_{ij}) \; \frac{\partial \, \Delta G}{\partial \, Nj} = 0$$

A procedure described in the literature as the Newton or Newton–Raphson method may be applied in order to solve the equations and to obtain numeral values. The computer calculations for the equilibrium data were described in the report of Combustion Engineering, Inc. (21).

203 The reaction of coal-char with the gases. The rate constant for the char reactions can generally be written in the Arrhenius form: $K = A \exp (E/RT)$ where E is the activation energy and the parameter A is the frequency factor and does depend on the number of molecules covering unit surface area. These values vary depending on the type of reaction and the carbon sample; for example, for the carbon-oxygen reaction it is from 20-80 Kcal/mole, for the carbon-steam reaction it is from 55-83 Kcal/mole [Isley et al. (14)] and for the carbon-carbon dioxide reaction it is from 26-84 Kcal/mole. Johnson (15) reported the kinetics of bituminous coal char gasification with gases containing steam and hydrogen.

The petrographic type and coal rank affects the char reactivity during gasification [Davis et al. (1)] so that the velocity constant for the coal type subjected to underground gasification should be determined experimentally. The manual of coal conversion fundamentals recently prepared by the Institute of Gas Technology presents a calculation procedure (using a char of a known reactivity factor) for the produced gas composition from a fluidized bed gasifier. However, for an average flame front velocity of about 0.1 cm per hr. in the underground gasification and for the resulting long residence time of char in a high temperature gasification zone, (30-130 hours) the char reactivity does not play a significant role.

The reaction of coal with steam and the resulting gas composition is defined by the kinetic of the two primary and two secondary reactions:

$$C + H_2O = CO + H_2 \tag{1}$$

$$C + 2 H_2O = CO_2 + 2 H_2 \tag{2}$$

$$CO_2 + C = 2 CO \tag{3}$$

$$CO + H_2O = CO_2 + H_2 \tag{4}$$
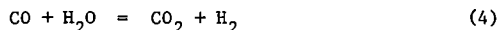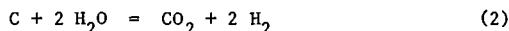
By denoting Z_i as the participation coefficient of the i reaction in the mixture, we would obtain [according to B. M. Derman (3)]:

$$Z_i = \frac{d (C x) V_i}{\Sigma d (C_x)} \quad \text{and (e.g.)} \quad \frac{dc^1}{dc^{111}} = \frac{2 Z_3 + Z_1 - Z_4}{Z_1 + 2 Z_2 + Z_1}$$

Experimental data [Ludin et al. (26)] show that the conversion reaction occurs downstream from gasification zone is catalyzed by the inorganic matter in the coal. Therefore, the modification of the gas composition due to this reaction should be included in the last stage of a computation.

204 A hybrid computer program was prepared by NASA (TMx-3403) that can solve chemical kinetic systems with many chemical species for either a flow or static reactor.

300 Energy balance and temperature profile calculation approach.

301 The general solid phase (coal-char) energy balance may be presented as follows:

[Thermochemical heat from reactions] + [heat input (output) by conduction] - [convective loss to flowing gas] + [Extended loss e.g. ash] = [Net heat accumulated in solid phase].

Analysing the mass balance, the change in an accumulation of solid phase may be obtained from the equation:

[Carbon used by oxygen] + [Carbon used by carbon dioxide] + [Carbon used by the reaction with steam] = – [Change of solid accumulation].

The primary combustion reaction rate is controlled by the oxygen supply. One dimensional peak temperature and temperature profile are a function of the following parameters: the total heat generated by carbon combustion reactions, the total heat losses and dissipated energy resulted by the coal conductivity, water heating and evaporation, convective heat transfer from solid to flowing gases, and heat losses in the leftover ash. The endothermic reactions, e.g., between the steam and char, are usually considered as a portion of the carbon combustion reactions. The approximated results may be obtained using the calorific value of coal instead of the heat reaction.

In the one dimensional energy balance the total heat of the various reactions would be expressed:

$$\sum_{i=1}^{n} \Delta H_i \frac{\partial x_i}{\partial time} \mu = total\ heat \tag{1}$$

where x_i is stochiometric coefficient of reaction and μ is a function of the solid phase which reacts with oxygen (carbon dioxide; steam).

320 We can now combine the heat transfer sink by conduction (solid) and the heat reaction representing uniformly distributed heat source and express it by the equation:

$$\frac{\partial}{\partial x} (K \frac{\partial t}{\partial x}) + \frac{\partial}{\partial y} (K \frac{\partial t}{\partial y}) + \frac{\partial}{\partial z} (K \frac{\partial t}{\partial z}) + \sum_{i=1}^{i=n} \Delta H_i \frac{\partial x_i}{\partial time} \mu = \rho c \frac{\partial t}{\partial time} \tag{2}$$

(t = temperature) This equation can be easily converted to the form containing the property $(\frac{K}{\rho c}) = \alpha$ which is the thermal diffusivity coefficient. Several authors (American and Russian) have confirmed that the temperature peak of coal combustion depends on this coefficient. However, the porous-capillary property of coal–char material requires further modification of the equation due to the convective transport associated with forced air and the gas flowing through the body. This should include the coolant mass flow (Gc) and the porosity of the material $(\frac{Cc}{Ke})$. For one dimensional conduction equation (2) becomes:

$$\frac{\partial^2 t}{\partial x^2} + \frac{Gc \cdot Cc}{Ke} \frac{dt}{dx} + \frac{\sum \Delta H_i \frac{\partial x_i}{\partial t} \mu}{K} = \frac{1}{\alpha} \frac{\partial t}{\partial time} \tag{3}$$

Depending on the boundary conditions various types of solution of this type of equation may be obtained. If we assume that the high temperature gasification zone may be represented as a porous plate cooled on our side, then the general solution of the equation (3) becomes:

$$\frac{t - t_x}{t_a - t_x} = \frac{Bi}{Bi + F} e^{-p\ (\alpha/s)} \tag{4}$$

where Bi is the Biot number and F is a Fourier number.

303 Further steps should include the heat losses by convection from the solid to the flowing gases. The significant portion of this type of heat loss is related to heating of the nitrogen and the water vapors.

The heat transfer from solid surfaces to the flowing gases and water vapor can be conveniently expressed in terms of a nondimensional Nusselt number, $Nu = \frac{hD}{K}$, where

h is the heat transfer coefficient, K is the thermal conductivity of the gas and D is a characteristic dimension. For turbulent flow, Nu = f (Re) where Re is a Reynolds number.

A significant difference of opinion exists as to whether or not a turbulent flow type occurs during the gasification in situ [Hahn & Debrand (13)]. It probably depends on the local circumstances of gasificaion such as cracks size, channeling, surface area of the channels, etc. Therefore a practical solution would include an estimation of this loss by the equation:

$$\frac{Q \text{ convective}}{V \text{ nitrogen}} = h \text{ (T average - T inlet)} \qquad (5)$$

where V nitrogen is the flow rate of nitrogen in the blast air; T inlet gas temperature, T average - temperature of gasification zone.

304 A significant effect of the ash content upon the peak temperature of gasification zone was observed experimentally. Some experimental data has shown that the exothermic reaction of ash formation does not compensate for the latent heat of the ash left in the gasification zone. The estimated heat losses would be proportional to the ash content in the coal and the rate of the coal combustion $(\frac{\Delta m}{\text{time}})$:

$$Q_{ash} = K_1 \cdot \Delta \text{ Ash content} \cdot \frac{\Delta m \text{ carbon}}{\text{time}} \qquad (6)$$

305 Based on the water heat balance, the heat use for the water evaporation and the water vapor latent heat, should be included. This heat would be proportional to the moisture content of the coal and the rate of the coal combustion:

$$Q_{water} = K_2 \Delta \text{ water content} \frac{\Delta m \text{ carbon}}{\text{time}}$$

306 The width and the rate of advancement of the gasification zone are proportional to the rate of the blast air. The coal combustion rate is also controlled by the supply of oxygen and in this contex, the oxygen supply rate is the only independent factor.

In the circumstances in which the water supply (influx) can be controlled, the ratio of total moisture/oxygen supply effects the following parameters:

a)   The equilibrium and the kinetics of the combustion reaction as well as changes in the balance of the thermochemical heat of the gasification reaction.

b)   The change of the temperature in the gasification zones due to the enthotermic reaction of steam decomposition and the heat sink is determined by the heat related to the water evaporation, latent heat of steam and heat loses to the strata.

The total solid phase energy balance would include the above mentioned interrelated expressions for the nonsteady heat transfer and the definition of the boundary conditions. The limitation of these calculations lie in the assumed boundary conditions. Further study is needed in this area.

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